STRUCTURE OF Si_n CLUSTER ANIONS: COMPARISON OF THEORY AND EXPERIMENT

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We have measured photoelectron spectra for silicon cluster anions with up to 50 atoms. For species with up to 20 atoms, the spectra have been compared with DFT simulations for a number of candidate low-energy geometries.[a] An excellent agreement with experiment specific to the lowest-energy Si_n anion geometries (Fig.1) validates the morphologies of medium-sized Si clusters based on the tricapped trigonal prism unit. HOMO-LUMO gaps do not decrease with increasing cluster size, but vary irregularly in the 1-2 eV range. The PES data for larger clusters with $n > 25$ reveal a peculiar electronic structure for Si_{33} and Si_{43} anions.

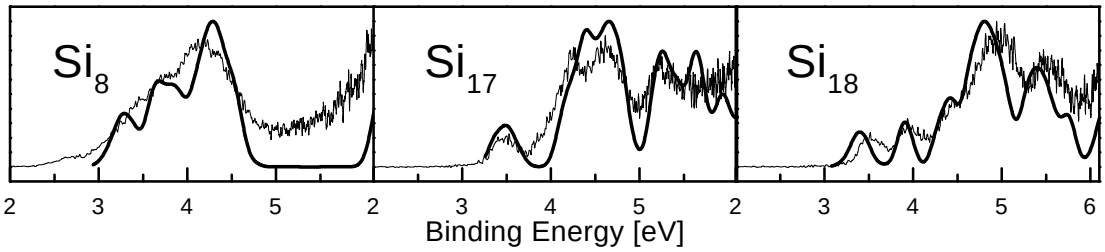

Fig.1: Comparison between simulated and measured PES spectra of Si_8, Si_{17}, and Si_{18}.

[a] A.A. Shvartsburg et al., J. Chem. Phys. **112** (2000)